

NANOMATERIALREGISTRY

**Anthony J. Hickey,
Alexander Tropsha, and Karmann Mills**
RTI International

Workshop on A Uniform Description System for Nanomaterials
Rockville, MD
June 10th, 2015

FEDERAL NANOTECHNOLOGY INITIATIVE

The NNI Coordinates R&D in nanoscale science, engineering, and technology



NNI

National Nanotechnology Initiative

NKI

Nanotechnology Knowledge Infrastructure
Thrust 4: Digital Information Infrastructure

NIH



Nanomaterial Registry Project

FEDERAL AGENCIES

- DoD
- DoE
- EPA
- FDA
- NASA
- NIH
- NIOSH
- NIST
- NSF
- OSHA
- ...

...cyber-toolbox, and data infrastructure that will shorten the time from research to new product development..

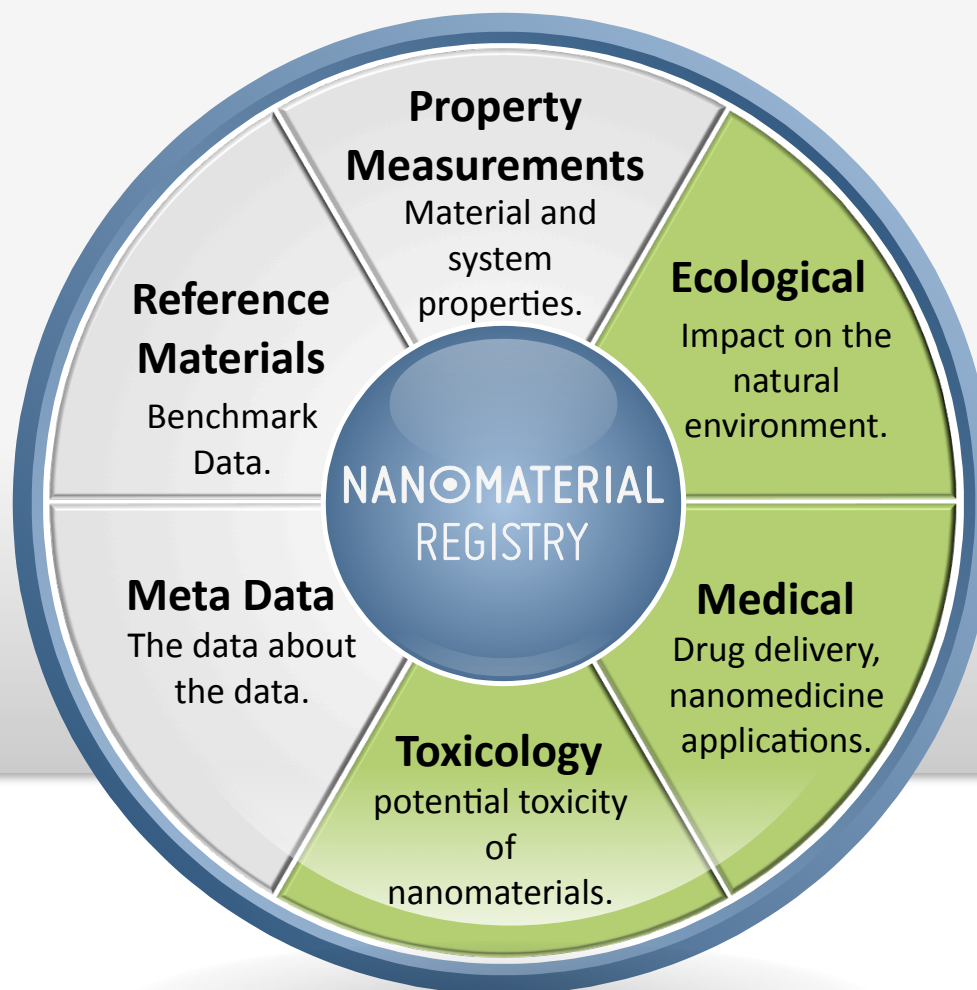
http://nano.gov/sites/default/files/pub_resource/nki_nsi_white_paper_-_final_for_web.pdf

NANOMATERIALREGISTRY

What you can expect to find in the Nanomaterial Registry

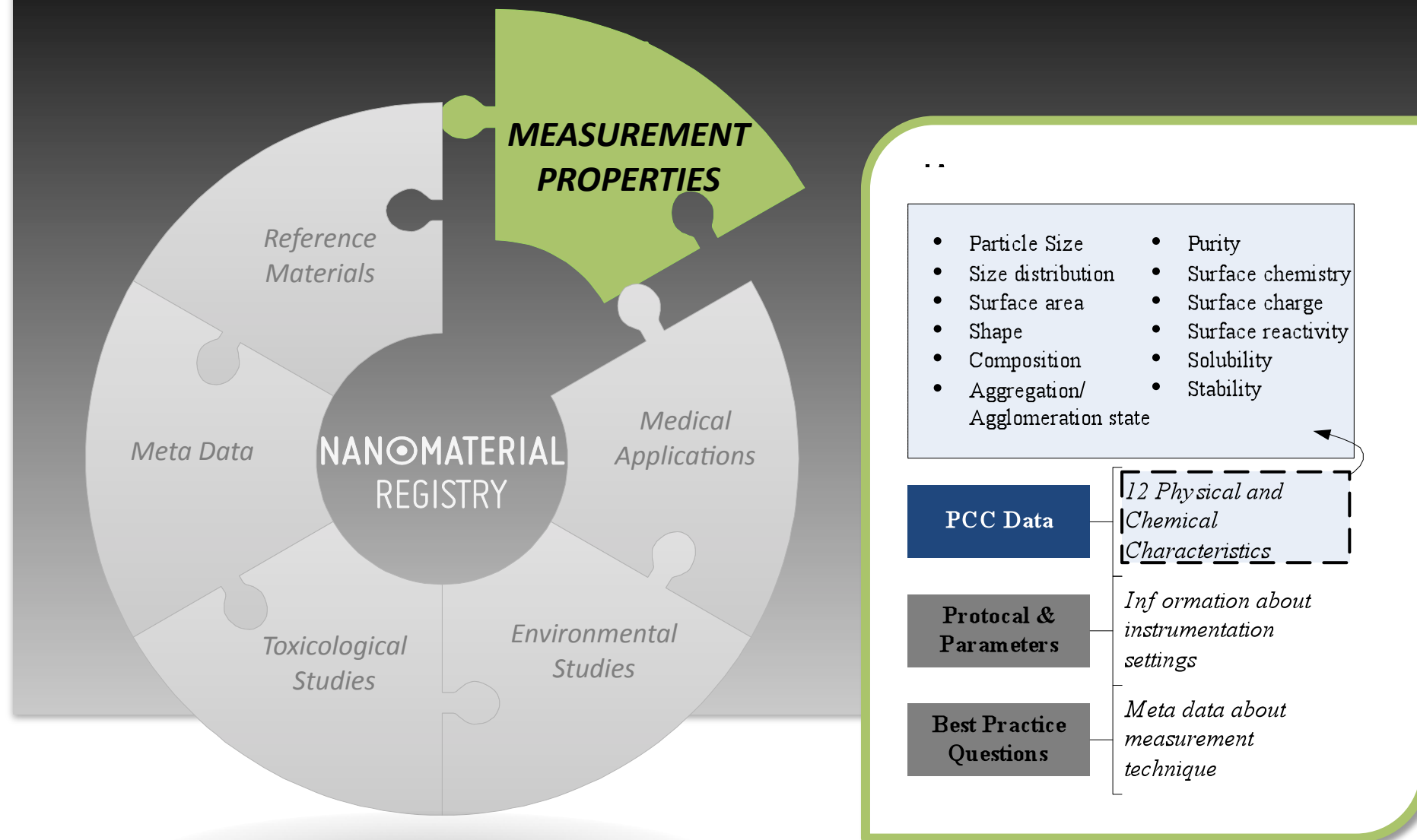
DATA DOMAIN

DOMAIN: CHARACTERIZATION + STUDY DATA



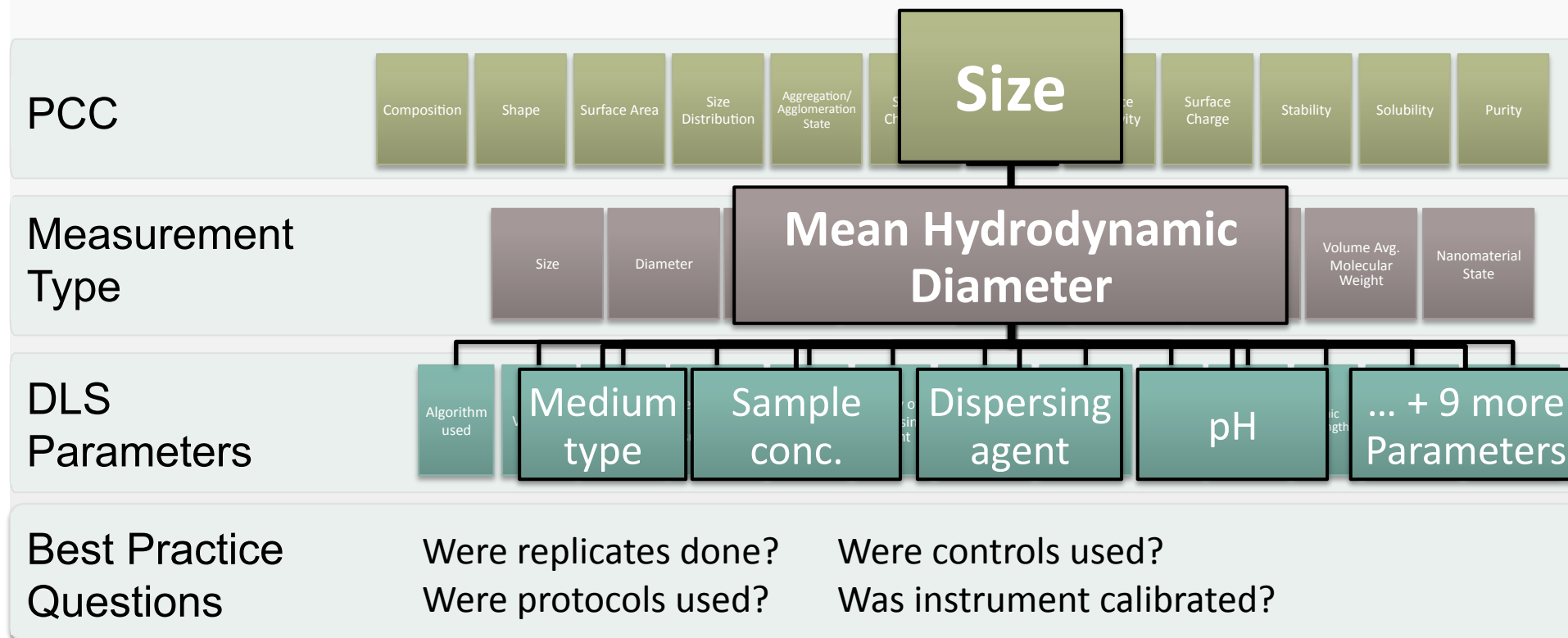
- ▶ **Validated** both programmatically and by a team of scientists
- ▶ **Integrated** through controlled vocabulary and data formatting
- ▶ **Relevant** growing body of data that is available to the public

LOOKING ACROSS THE CHARACTERIZATION DATA



A **controlled vocabulary** of PCC & measurands have been identified (<https://www.nanomaterialregistry.com/resources/Glossary.aspx>)

Minimal Information About Nanomaterials



DATA RECORDS IN THE REGISTRY

PDF (TEXT)

PEER REVIEWED
LITERATURE

ORIGINAL RESEARCH PUBLICATION

[Nanomedicine \(Lond\)](#). 2012 Aug;7(8): 1197-209. doi: 10.2217/nnm.12.18. Epub 2012 May 14.

Silver nanoparticles do not influence stem cell differentiation but cause minimal toxicity

[Samberg ME](#), [Loboa EG](#), [Oldenburg SJ](#), [Monteiro-Riviere NA](#).

DATA IS
CURATED
INTO THE
DATABASE



TWO UNIQUE DATA RECORDS

NR1130, NR1131

- MULTIPLE COMPOSITIONS? No
- MULTIPLE SIZES? Yes: 10 nm, 20 nm
- MULTIPLE MANUFACTURERS? No

FROM JOURNAL TEXT: “....Two solutions of spherical **Ag-NPs** were obtained from **NanoComposix** (CA, USA), each at Ag-NP concentration of 1.00 mg/ml with diameters of **10 and 20 nm**.....”

PARSED DATA

NANOMATERIAL
REGISTRY

NANOMATERIAL CHARACTERIZATION

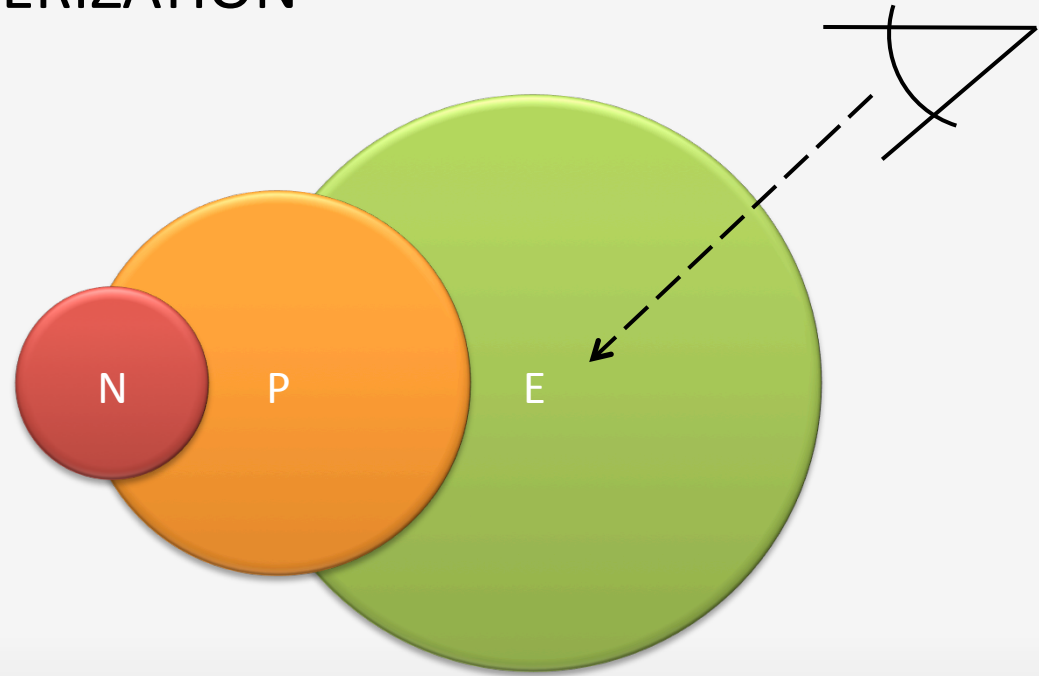
Individual nanoparticles exist in

- **POPULATION** (P) of particles
- **ENVIRONMENT** (E)



Observed Characteristic =

$$f(P,E)$$

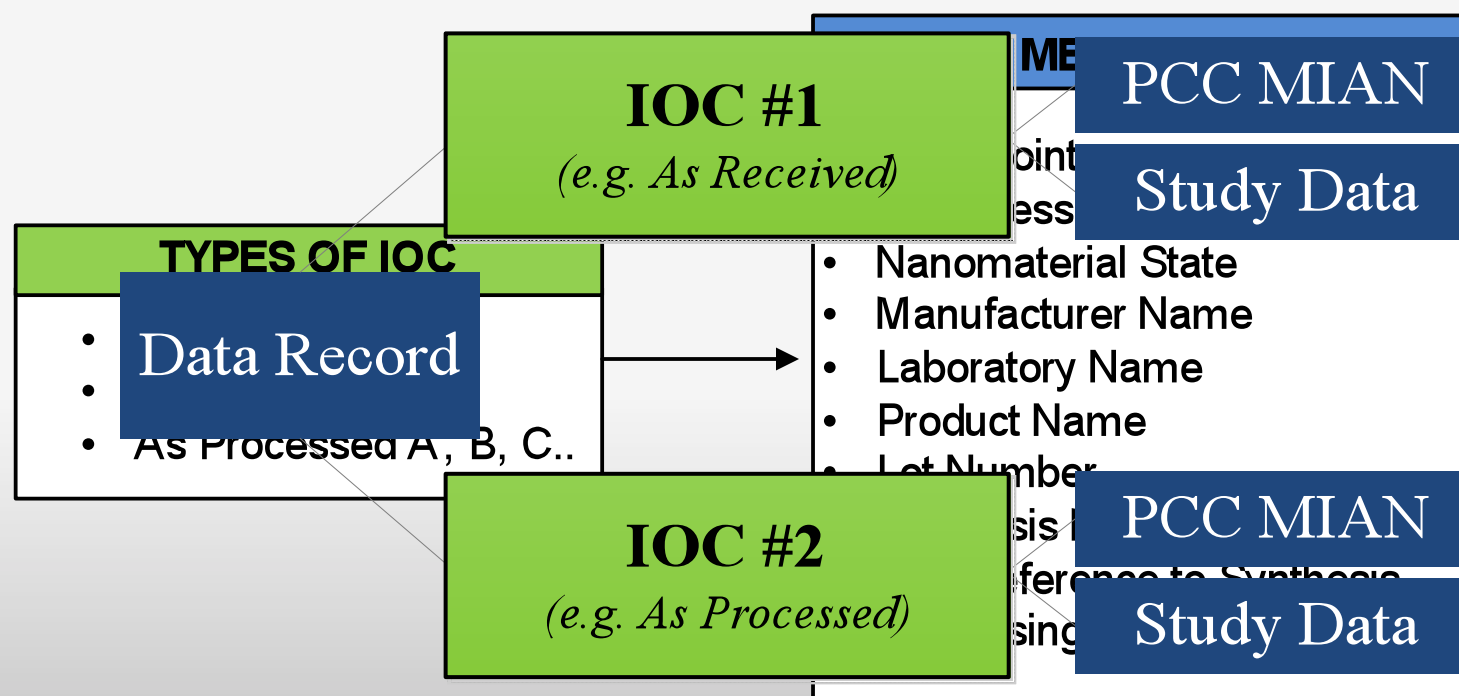


Additional considerations:

- Individual Particle
- Population/sampling
- Environment
- Time
- Measurement technique













$$= f(P,E,T,M...)$$

DATA INSTANCE OF CHARACTERIZATION



DATA RECORD

NM CHARACTERIZATION *Example Record: NR1130*

✓  Composition	MIAN PCC Information from NR1130: Material Type: Metal Molecular Identity: Silver	IOC = As Synthesized
✓  Size		
 Size Distribution	Primary Particle Size: 10 nm Core Size: 5 nm (Gold Core)	IOC = As Processed A suspended in water (for DLS)
✓  Shape		
 Aggregation/Agglomeration State	Mean Hydrodynamic Diameter: 21.7 ± 0.3 nm <i>Dynamic Light Scattering</i>	IOC = As Processed B Dried (for TEM)
 Surface Area		
✓  Surface Charge	Zeta Potential: -40.6 ± 0.4 mV <i>Electrophoretic Light Scattering</i>	IOC = As Processed B Dried (for TEM)
 Surface Chemistry		
 Surface Reactivity	Mean Diameter: 7.2 ± 1.2 nm <i>Transmission Electron Microscopy</i>	IOC = As Processed B Dried (for TEM)
 Purity		
 Solubility	Dimensions in the Nanoscale: 3D <i>Transmission Electron Microscopy</i>	IOC = As Processed B Dried (for TEM)
 Stability		



TYPES OF
CHARACTERIZATION

MEASUREMENT VALUES
& TECHNIQUES

ENVIRONMENTS &
TIME POINTS

LOOKING ACROSS TECHNIQUES



Particle size is
frequently reported
without technique

(LOW DATA QUALITY RATING)



**Dynamic light
scattering** is the
most curated
technique

Techniques used to measure
particle size

LOOKING ACROSS PARAMETERS

► **Solvent Type** is the most frequently reported parameter for DLS

Other DLS parameters that are collected, but not shown here, include

- ✓ **scattering angle**
- ✓ **wave length**
- ✓ **index of refraction**

DETAILS PAGE META DATA

NR963

NR Descriptor: Au NP

Information for this nanomaterial was curated from National Institute of Standards and Technology.

Original Publication(s): Not reported

Information reported: [PCC Characterization?](#) Yes [Environmental Interactions?](#) No

CURATED DATA BASED ON INSTANCE OF CHARACTERIZATION

AS RECEIVED

AS PROCESSED A

AS PROCESSED B

[make a comment](#)

AS RECEIVED

Nanomaterial State: liquid suspension

Manufacturer: National Institute of Standards & Technology

Product Name: Reference Material 8011

Synthesis Method: citrate reduction

PHYSICO-CHEMICAL CHARACTERISTICS

BIOLOGICAL INTERACTIONS

ENVIRONMENTAL INTERACTIONS

Particle Size

Mean Hydrodynamic Diameter: 13.5 nm +/- 0.1 nm
Dynamic Light Scattering

Mean Hydrodynamic Diameter: 9.1 nm +/- 1.8 nm
Small Angle X-Ray Scattering

Mean Hydrodynamic Diameter: graphically represented
Intensity Weighted Field Flow Fractionation

Composition

OVERALL NANOMATERIAL

Molecular Identity: UV-Visible Spectroscopy

Lambda Max: 517 nm

COATING

CORE

Best Practice Questions

BEST PRACTICES

Instrument Manufacturer: Malvern

Instrument Model: Zetasizer Nano ZS

Raw Data Provided: Not reported

Proper Controls Used: Not reported

Instrument within Calibration: Yes

Number of Replicates: 40

Protocol Reported: Not reported

Protocol Citation: ISO 13321:1996(E)

Protocol Modifications: Not Reported

Measurement Parameters

PROTOCOL & PARAMETERS

Temperature of Suspension: 20 +/- 0.1 C

Algorithm Used: cumulants

Viscosity: 1.0031 mPa*s

Solvent/Medium Type: water

Dispersing Agent: NaCl

Concentration of Dispersing Agent: 2 mM

Sample Concentration: diluted 6-fold

Sonication/Milling Power: none

Sonication/Milling Time: none

NIST Reference Material 8011 – Citrate stabilized Au NP





NANOMATERIALREGISTRY

Compliance Levels in the Nanomaterial Registry

DATA QUALITY

DATA QUALITY METRIC

The Nanomaterial Registry's **COMPLIANCE LEVEL FEATURE** provides a **METRIC** on the **QUALITY** of characterization of a nanomaterial entry

Compliance Level	Score	Medal
Gold	76-100	
Silver	51-75	
Bronze	26-50	
Merit	0-25	

COMPLIANCE LEVELS are broken into **MERIT**, **BRONZE**, **SILVER**, and **GOLD** and represent increasing quality of characterization based on our evaluation criteria

↓
A COMPLIANCE LEVEL SCORE is a quantitative value calculated by an algorithm

MORE INFORMATION: <https://www.nanomaterialregistry.com/about/HowIsComplianceCalculated.aspx>

DATA QUALITY METRIC

YOUR CURRENT KEYWORD SEARCH

☐ Also search within words, phrases, or formulas.

NARROW YOUR SEARCH

☐ Size MORE >

☐ Agg/Agg State

☐ Size Distribution

☐ Surface Area MORE >

☐ Shape MORE >

☐ Composition MORE >

☐ Purity MORE >

☐ Surface Charge MORE >

☐ Surface Chemistry

☐ Surface Reactivity

☐ Solubility MORE >

☐ Stability

☐ Biological MORE >

☐ Environmental MORE >

REVISE SEARCH >

16 RESULTS FOUND FOR TiO2

COMPLIANCE LEVELS

★ Gold

◆ Silver

🏅 Bronze

🏆 Merit

	PCC COMPLIANCE	PARTICLE SIZE	SIZE DISTRIBUTION	AGGREGATION / AGGLOMERATION STATE	SURFACE AREA	SHAPE	COMPOSITION	PURITY	SURFACE CHARGE	SURFACE CHEMISTRY	SURFACE REACTIVITY	SOLUBILITY	STABILITY	BIOLOGICAL	ENVIRONMENTAL
NR68 - TiO2 NF	🏅	🏅		◆	★	★									
NR91 - TiO2 NP	🏅		◆	★	★	★									
NR467 - TiO2 NP	🏅	◆			★	★									
NR809 - TiO2 NP	🏅	◆		★	★	★									
NR810 - TiO2 NP	🏅	🏅		★	★	★									
NR811 - TiO2 NP	🏅	🏅		★	★	★									
NR932 - TiO2 NP	🏅				★	★									
NR933 - TiO2 NP	🏅				★	★									
NR968 - TiO2 NP	🏅	★	◆	★	★	★	★	★	🏅						
NR1076 - TiO2 NP	🏅	◆			★	★									
NR1102 - TiO2 NP	🏅	🏆			★	★									
NR1278 - TiO2 NP	🏅	◆	★	★	★	★									

COMPLIANCE LEVELS

★ Gold

◆ Silver

🏅 Bronze

🏆 Merit

Yes Yes

No No

No No

No No

No No

No No

No No

No Yes

No Yes

No No

Compare Selected >

DATA QUALITY METRIC

Records with more specific measurement data are awarded more points than those with less specific data

Scenario 1	Scenario 2	Scenario 2	Scenario 4
Size= 37.5 nm	Size= 37.5 nm Mean Hydrodynamic Diameter	Size= 37.5 nm Mean Hydrodynamic Diameter Dynamic Light Scattering Malvern ZetaSizer Nano ZS	Size= 37.5 nm Mean Hydrodynamic Diameter Dynamic Light Scattering Malvern ZetaSizer Nano ZS 11 of 12 measurement parameters reported Protocol: ASTM E2490 - 09
Merit	Bronze	Silver	Gold

Algorithm

Assigns weights to each value that appears in a curated record

$$CL_{PCC} = \sum_{Measurements} \left\{ \frac{\sum_G M_G * P_G}{\sum_G M_G * W_G} \right\}$$

NAN⊙MATERIALREGISTRY

THANK YOU!

www.nanomaterialregistry.org

www.nanomaterialregistry.com

nanoregistry@rti.org